Methyl pivalate
598-98-1 | DTXSID4027234

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -92.2 °C

Global applicability domain: Inside

Local applicability domain index: 9.36e-01

Confidence level: 8.88e-01

Nearest Neighbors from the Training Set

Image not found
Butan-2-yl acetate
Measured: -98.9
Predicted: -92.5

Image not found
Isobutyl acetate
Measured: -98.8
Predicted: -92.5

Image not found
Ethyl isobutyrate
Measured: -88.2
Predicted: -92.3

Image not found
Butyl acetate
Measured: -78.0
Predicted: -83.6